

12.0 Data Analysis and Calculations

Data analysis is performed using appropriate reference spectra whose concentrations can be verified using CTS spectra. Various analytical programs (References 10 and 11) are available to relate

sample absorbance to a concentration standard. Calculated concentrations should be verified by analyzing spectral baselines after mathematically subtracting scaled reference spectra from the sample spectra. A full description of the data analysis and calculations may be found in the FTIR

Protocol (sections 4.0, 5.0, 6.0 and appendices).

12.1 Calculated concentrations in sample spectra are corrected for differences in absorption pathlength between the reference and sample spectra by

$$C_{\text{corr}} = (L_r / L_s) \times (T_s / T_r) \times (C_{\text{calc}}) \quad (5)$$

Where:

C_{corr} = The pathlength corrected concentration.

C_{calc} = The initial calculated concentration (output of the multicomponent analysis program designed for the compound).

L_r = The pathlength associated with the reference spectra.

L_s = The pathlength associated with the sample spectra.

T_s = The absolute temperature (K) of the sample gas.

T_r = The absolute temperature (K) at which reference spectra were recorded.

12.2 The temperature correction in equation 5 is a volumetric correction. It does not account for temperature dependence of rotational-vibrational intensities. Whenever possible, the temperature correction should be used in the test to minimize the calculated error in the measurement (FTIR Protocol, appendix D). Additionally, the analytical region chosen for the analysis should be sufficiently broad to minimize errors caused by small differences in relative line intensities between reference spectra and the sample spectra.

13.0 Method Performance

A description of the method performance may be found in the FTIR Protocol. This method is self validating provided the results meet the performance specification of the QA spike in sections 9.0 through 9.3 of this method.

14.0 Pollution Prevention

This is a gas phase measurement. Gas is extracted from the source, analyzed by the instrumentation, and discharged through the instrument vent.

15.0 Waste Management

could not find this publication. Not at EPA. Not at NTIS. No hit's in Google search.

2. "Evaluation of HCl Measurement Techniques at Municipal and Hazardous Waste Incinerators," S.A. Shanklin, S.C. Steinsberger, and L. Cone, Entropy, Inc. Prepared for U.S. Environmental Protection Agency, Research Triangle Park, NC. NTIS Report No. PB89-220586. (1989).

3. "Fourier Transform Infrared (FTIR) Method Validation at a Coal Fired-Boiler," Entropy, Inc. Prepared for U.S. Environmental Protection Agency, Research Triangle Park, NC. EPA Publication No. EPA-454/R95-004. NTIS Report No. PB95-193199. (1993).

4. "Field Validation Test Using Fourier Transform Infrared (FTIR) Spectrometry To Measure Formaldehyde, Phenol and Methanol at a Wool Fiberglass Production Facility." Draft. U.S. Environmental Protection Agency Report, Entropy, Inc., EPA

Contract No. 68D20163, Work Assignment I-32.

5. Kinner, L.L., Geyer, T.G., Plummer, G.W., Dunder, T.A., Entropy, Inc. "Application of FTIR as a Continuous Emission Monitoring System." Presentation at 1994 International Incineration Conference, Houston, TX. May 10, 1994.

6. "Molecular Vibrations; The Theory of Infrared and Raman Vibrational Spectra," E. Bright Wilson, J.C. Decius, and P.C. Cross, Dover Publications, Inc., 1980. For a less intensive treatment of molecular rotational-vibrational spectra see, for example, "Physical Chemistry," G.M. Barrow, chapters 13, 14, and 14, McGraw Hill, Inc., 1979.

7. "Laboratory and Field Evaluations of Ammonium Chloride Interference in Method 26," U.S. Environmental Protection Agency Report, Entropy, Inc., EPA Contract No. 68D20163, Work Assignment No. I-45.

8. 40 CFR 63, appendix A. Method 301—Field Validation of Pollutant Measurement Methods from Various Waste Media.

9. "Fourier Transform Infrared Spectrometry," Peter R. Griffiths and James de Haseth, Chemical Analysis, 83, 16-25, (1986), P.J. Elving, J.D. Winefordner and I.M. Kolthoff (ed.), John Wiley and Sons.

10. "Computer-Assisted Quantitative Infrared Spectroscopy," Gregory L. McClure (ed.), ASTM Special Publication 934 (ASTM), 1987.

11. "Multivariate Least-Squares Methods Applied to the Quantitative Spectral Analysis of Multicomponent Mixtures," Applied Spectroscopy, 39(10), 73-84, 1985.

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